PERGAMON

Applied Mathematics Letters 14 (2001) 413–418

Applied Mathematics Letters

www.elsevier.nl/locate/aml

Hamiltonian Circuited Simulations of Elliptic Partial Differential Equations Using a Spark

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(Received and accepted May 2000)

Communicated by E. L. Ortiz

Abstract—The finite-difference schemes give linear relations of the unknowns. Iterative simulations of partial differential equations are seen as iterative processes, and hence, an attempt is made to treat the points to be simulated as vertices of a graph. One way to pass through the vertices once and only once in an iteration is to simulate in a Hamiltonian circuit. Thus, in this paper, Hamiltonian circuited simulations of an elliptic partial differential equation using a spark as a means of providing linear relationship between unknowns are given. The Hamiltonian circuit in use enables the decomposition of the coefficient matrix into two blocks such that the simulated points are decomposed into two disjoint sets. We appreciate that the simulations now are done in parallel involving much reduced simulation points.

Keywords—Finite-difference sparks, Hamiltonian circuits, Elliptic partial differential equations.

1. INTRODUCTION

The system of equations accruing from finite-difference modelling of partial differential equations is very large indeed, especially when finer meshes are used. The system of equations is obtained after a finite-difference scheme with implied numbering system is specified. The finite-difference schemes are means to correlate the unknowns among themselves and we categorize them as stars or diamonds or sparks.

Large systems of equations accruing from a finite-difference scheme are usually banded or blocked. Attempts to gain efficiency in the numerical simulations of partial differential equations have been made via complete or incomplete factorization of Dupont *et al.* [1] or Stone [2] or Meijerink and van der Vorst [3,4]. Tridiagonal coefficient matrices are most welcome as they alleviate computer storage problems. So, it is desirable to split the matrix into the tridiagonal form or at least into those with small bandwidths. Such attempts are associated with Douglas [5] and Peaceman and Rachford [6]. Instead of splitting and factorization, the work of Evans [7–9] and Abdullah [10–13] involves partitioning.

0893-9659/01/$ - see front matter Typeset by $\mathcal{A}\mathcal{M}\mathcal{S}$-TEX
PII: S0893-9659(00)00170-1

Now that the methods for solving large sparse systems are iterative in nature, we are inclined to treat simulation points as vertices of graphs. They, in fact, form an ugly looking thing known as a complete graph. The best way to go through the vertices once in an iteration is by way of a Hamiltonian circuit. With it, an appropriate finite-difference star will set in, thus giving rise to a certain algebraic structure in the matrix coefficients of the unknowns.

Section 2 explains fundamental concepts of graphs and gives a generation of a Hamiltonian circuit which enables decomposition of subspace of the simulated points. Section 3 outlines the finite-difference "spark" modelling for the elliptic partial differential equation used in our numerical experiments. Section 4 presents algebraic structures for matrix coefficients of Hamiltonian circuited simulated points of the nine-point rotated finite-difference "spark". Results of our numerical endeavors are presented in Section 5.

2. ON HAMILTONIAN CIRCUITS

Simulations of points for partial differential equations are sequential processes and they constitute vertices of a graph. A graph G is a pair $\{V(G), E(G)\}$, where $V(G)$ is a finite nonempty set of elements called vertices and $E(G)$ is a finite set of distinct unordered pairs of distinct elements of $V(G)$ called edges. The edge $\{v, w\}$ is denoted by vw, where v and w are vertices of G. If $e = vw$ is an edge of G, then e is said to join the vertices v and w, and these vertices are then said to be adjacent. If e is incident to v and w, then w is a neighbor of v. The neighborhood of v denoted by $N(v)$ is the set of all vertices of G adjacent to v. Two edges of G incident to the same vertex are called adjacent edges.

For each vertex of a graph G, the number of edges incident to v is called the degree of v, denoted by $d(v)$. If all the vertices of G have the same degree, G is said to be a regular graph. A graph in which every two vertices are adjacent is called a complete graph, i.e., every vertex is adjacent to every other vertex. A graph G is connected if there is a path joining each pair of vertices of G. A graph G may be disconnected by removing various sets of vertices. Any such set of vertices will be called a disconnecting vertex set. A sequence of edges of the form $v_0v_1, v_1v_2, \ldots, v_{r-1}v_r$ (or $v_0v_1, \ldots, v_r$) is called a walk of length r from v_0 to v_r. v_0 is called the initial vertex of the walk. v_r is called the terminal vertex. If these edges are all distinct, the walk is called a trail and if vertices $v_0, v_1, \ldots, v_r$ are also distinct, then the walk is called a path. A walk in which the vertices $v_0, v_1, \ldots, v_r$ are all distinct except for v_0 and v_r is called a circuit (or cycle). A way to go through the vertices of a graph once and only once in an iteration is via Hamiltonian circuits.

2.1. Generation of a Hamiltonian Circuit

Identifying simulated points as vertices of a complete graph where every vertex is adjacent to every other vertex and using the theorem due to Pósa which characterizes a class of Hamiltonian graphs, the graph is Hamiltonian, i.e., a Hamiltonian circuit can be found for the graph, i.e., the unknowns can be simulated in a Hamiltonian circuited ordering. Here we generate a number of Hamiltonian circuited orderings for the unknowns. Suppose that the graph consists of 64 vertices, i.e., the number of unknowns is 64, where the finite domain of definition of the partial differential equation at hand is made up of eight points for each of the eight rows in the y-axis. A way to get a Hamiltonian circuit is first to colour the vertices with four different colours so that no nearest neighbors are of one colour. Considering each of the eight rows as having eight points, we colour the vertices as follows.

For the first row, the first four points are coloured with four different colours. The colours are repeated for the next four points. For the second row, the first point is coloured with the third colour used to colour the third point of the first row. The second point is coloured with the colour used to colour the fourth point of the first row. In general, the last two colours are

used to colour the first two colours of the first two points of successive rows. For example, the 64 points are coloured as follows:

y w r b y w r b
r b y w r b y w
y w r b y w r b
r b y w r b y w
y w r b y w r b
r b y w r b y w
y w r b y w r b
r b y w r b y w,

where r denotes the "red" colour, b denotes "black", y denotes "yellow", and w denotes "white".

Now, starting with the first point with the colour "red", the program searches a "white" around it, then a "yellow", and finally a "black" and the search continues with these four colours horizontally. Thus, two rows are considered at any one time. The forward trip sees the repetition of the above-said search which dwindles between any two rows. When the search reaches the final point on the eighth row, the return trip takes place. The search starts with the last point on the seventh row which has a "white". The program now looks for a "red" around it. From here, this point seeks a "black" and then with this, a "yellow". The pattern search is repeated horizontally until the point where the search has found the final "yellow" on the second row, whence the program terminates with a Hamiltonian circuited sequence for the points to be simulated.

3. FINITE-DIFFERENCE "SPARK" MODELLING OF THE POISSON PROBLEM ON A SQUARE DOMAIN

This section outlines the finite-difference "spark" modelling for an elliptic partial differential equation. It first defines the Poisson problem which we have solved in this paper. Then the finite-difference "spark" approximation for the Laplacian term is given.

3.1. The Poisson Problem in Two Space Dimensions

The Poisson equation involving two space dimensions is given by

$$u_{xx} + u_{yy} = f(x, y), \qquad \text{for } (x, y) \in \Omega, \tag{3.1}$$

or in terms of the Laplacian operator, it is stated as

$$\nabla^2 u = f(x, y), \tag{3.2}$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial y^2}$ denotes the Laplacian operator.

The domain Ω over which the Poisson equation (3.1) is defined is the unit square in the x-y-plane, i.e.,

$$\Omega = \{(x, y) \mid 0 < x, y < 1\}.$$

For the complete Poisson problem, the boundary condition used is of the Dirichlet form

$$u(x, y) = g(x, y), \qquad \text{on } \partial\Omega. \tag{3.3}$$

3.2. Of Finite-Difference Stars or Diamonds or Sparks

To solve the Poisson problem numerically, a grid structure is imposed on the domain over which the partial differential equation is defined. Then a relation is obtained among the points. The relations which are feasible with the Hamiltonian circuit we generated in Section 2 are either the five-point star, the nine-point diamond, or the nine-point spark. They are diagrammatically given in Figure 1a, 1b, and 1c, respectively.

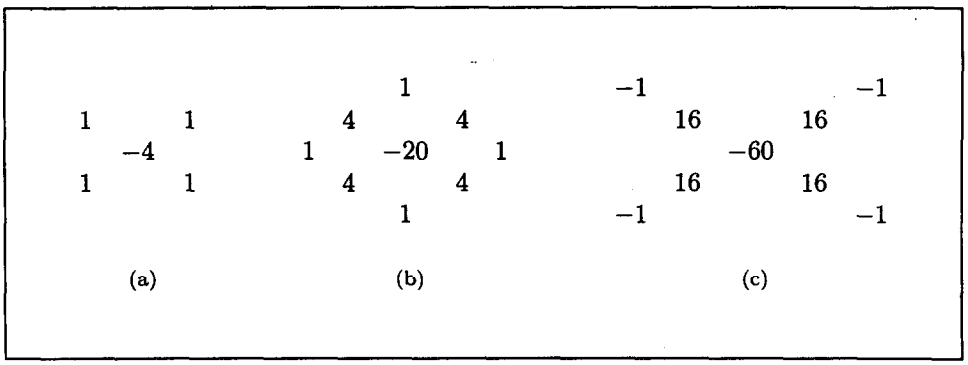

Figure 1. Of stars, diamonds, and sparks.

4. THE MATRIX COEFFICIENT RESULTING FROM THE NINE-POINT SPARK

When the Hamiltonian circuited unknowns are correlated by the nine-point finite-difference spark of Figure 1c, the coefficient matrix for half the number of unknowns takes the form given in Figure 2, where A_1 is a tridiagonal matrix with diagonal elements having the value -60 and off-diagonal elements having the value 16 whilst B_1 is the matrix

$$B_1 = \begin{bmatrix} & & -1 & & & & & & \\ 16 & & 16 & -1 & & & & & \\ -1 & & & & -1 & & & & \\ & -1 & 16 & & 16 & -1 & & & \\ & & -1 & & & & -1 & & \\ & & & -1 & 16 & & 16 & -1 & \\ & & & & -1 & & & & \\ & & & & & -1 & 16 & & \end{bmatrix}.$$

Table 2.

Matrix Size	Omega	Number of Iterations	Vectorial CPUs	Sequential CPUs
8 × 8	1	21	7.389e−3	1.418e−2
	1.2 ∼ 1.25	12	4.228e−3	8.105e−3
32 × 32	1	198	1.8572	3.26
	1.6	61	0.573	1.003
	1.65	51	0.479	0.839
	1.7	54	0.508	0.89
64 × 64	1	618	24.704	43.0
	1.75	129	5.15	8.97
	1.8	99	3.963	6.883
	1.85	159	6.36	11.057

5. SOME HAMILTONIAN CIRCUITED SIMULATION EXPERIMENTS

Some experiments on Hamiltonian circuited simulations of elliptic partial differential equations are reported in Table 1 for matrix sizes 8 × 8, 32 × 32, and 64 × 64. The experiments are

$$\begin{bmatrix} A_1 & B_1 & & \\ B_1^\top & A_1 & B_1 & \\ & B_1^\top & A_1 & B_1 \\ & & B_1^\top & A_1 \end{bmatrix}$$

Figure 2. The coefficient matrix derived from the "spark".

Table 1.

Matrix Size	Omega	Number of Iterations	Vectorial CPUs	Sequential CPUs
8 x 8	1	18	7.88e−4	2.995e−3
	1.05	15	6.597e−4	2.497e−3
	1.1	14	6.178e−4	2.334e−3
32 x 32	1	45	2.94e−2	0.1199
	1.15 ~ 1.2	32	2.095e−2	8.53e−2
64 x 64	1	72	0.188	0.76
	1.15	55	0.143	0.581
	1.2	52	0.135	0.549
	1.25	57	0.148	0.602

carried out using the Gauss-Seidel iterative method and repeated with several omega around the optimum omega parameter of the successive over relaxation method. Both sequential and vectorized processing modes are used in the experiments. The results are compared with those in Table 2 obtained by the method reported in [10] and using the finite-difference diamond. Both the diamond and the spark are $O(h^4)$ approximants to the Laplacian term of the Poisson equation when the $f(x, y)$ of equation (3.1) is harmonic. The spark is an $O(h^4)$ approximant to the Laplacian term of the Poisson equation when the $f(x, y)$ of equation (3.1) is nonharmonic, that is, the spark does not exhibit "amphibious" characteristic.

6. CONCLUSIONS

The Hamiltonian circuit provides a guide as to which unknowns are to be simulated before which unknowns. The algebraic structures are greatly influenced by the Hamiltonian circuit. Also affected by the Hamiltonian circuit is the use of finite-difference stars or diamonds. This particular Hamiltonian circuit has decomposed the space of unknowns into two subspaces. The results self-express the better performance obtained in using the "spark".

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